Contribution ID: **39** Type: **invited**

Point-Defect-Induced Metastable Phase Diagrams

Monday 26 May 2025 12:10 (30 minutes)

Excess lattice point defects can drive phase transformations, alter phase selection, or even lead to the formation of new phases. The removal of these defects serves both as a mechanism for accommodating precipitate eigenstrain and as a driving force for semi-coherent precipitation [1].

We present a thermodynamic framework for point-defect-induced precipitations, considering both precipitate eigenstrain and the Gibbs free energy associated with point defect formation. Additionally, we introduce the concept of a volume-constrained metastable phase diagram to rationalize phase selection in model alloys subjected to irradiation.

To compute these metastable phase diagrams, we rely on lattice parameters and CALPHAD databases, which provide the Gibbs free energy of equilibrium phases. For calculating the Gibbs free energies of point defects and phase formation in cases where reliable thermodynamic data are lacking, we develop statistical physics methods. These methods extract short-range order (SRO) contributions from ab initio random energy sampling [2,3]. This approach allows us to account for local atomic arrangements, leading to more accurate predictions of defect energetics, phase stability and metastability.

References

[1] Maylise Nastar, Lisa Belkacemi, Estelle Meslin, Marie Loyer-Prost, Commun. Materials 2 (2021), 32.
[2] T. Schuler, M. Nastar, K. Li, C.C. Fu, Towards Accurate Thermodynamics from Random Energy Sampling, Acta Mat 281 (2024) 120305
[3] K. Li, T. Schuler, C. C. Fu, M. Nastar, Vacancy Formation Free Energy in Concentrated Alloys: Equilibrium vs. Random Sampling, Acta Mat. 1 (2024) 120274

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Session Classification: invited